Booster Space Charge Modeling/Simulations Review

September 17, 2003

The results of a Booster Space Charge Modeling/Simulations review are reported. It was an internal Fermilab review organized by the Computing Division. The topic was a major project to simulate particle beam behavior, including a full three-dimensional treatment of space charge effects, in circular accelerators such as the Fermilab Booster.

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At the beginning of the review, the committee received the following “Abstract of the Work” to be reviewed:

> *The Advanced Accelerator Simulation Project, which is a multi-laboratory collaboration effort, is funded by the DOE SciDAC program. The goal of the project is to develop a suite of scalable and portable simulation software that can be used to solve challenging problems in accelerator design, analysis and optimization.*
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> *Fermilab physicists on the project have concentrated their efforts on modeling space charge effects in circular machines, specifically in the FNAL Booster, for high intensity operation scenarios where the effects are extremely important. The current program has focused on modeling of the Booster as well as performing beam studies with the machine. Data and simulations are compared in an attempt to both validate the model as well as to understand the performance of the Booster. In the process of carrying out the program, the Ion Profile Monitor, which is essential for understanding the evolution of the beam during the Booster cycle has been calibrated.*
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> *Modern software techniques have been introduced into the beam-modeling package, Synergia. Synergia re-uses existing beam physics codes, spans multiple languages, and provides an extensible framework. The code has a flexible human interface based on python and a portable build system which uses the GNU Autotools.*

On May 27th, the committee heard a series of presentations according to the following agenda:

* *Presentation of Charge - Pushpa Bhat*
* *Overview of the Project - Panagiotis Spentzouris*
* *Technical Implementation/Code Development - Jim Amundson*

** Applications and Plans - Panagiotis Spentzouris*
** Q & A*

In addition, the committee had access to project documents contained on this web page:

http://cepa.fnal.gov/psm/aas/Advanced_Accelerator_Simulation.html

The following documents in the Beams Documents Database, <http://beamdocs.fnal.gov/>, were also made available:

> Beams-doc-495-v2
> Beams-doc-581-v1
> Beams-doc-499-v1
> Beams-doc-498-v1
> Beams-doc-497-v1
> Beams-doc-496-v1
> Beams-doc-615-v1
> Beams-doc-616-v1

The charge to the committee consisted of the following items:

(1) Are the simulation techniques used in Synergia appropriate for evaluating space charge in the Booster and other circular machines?

(2) A well planned validation with data is critical for any simulation program. Has the validation program using Booster IPM data resulted in a useful test of the Synergia simulation package?

(3) Have sufficient beam studies with the Booster been made?

(4) Are the extrapolations to high intensity operation scenarios valid?

(5) Is the software suite user-friendly and efficient?

(6) Please comment on the plans for further simulations and studies.

General remarks

A few general remarks are in order before responding specifically to the charge.

Charged particle beams generate electric and magnetic fields that act back upon the particles in the beam, causing so-called space charge effects. Except in the trivial case of an unbunched cylindrical beam of uniform density, the forces resulting from these fields are nonlinear. These intensity-dependent nonlinear forces can disrupt the beam in a synchrotron via a variety of mechanisms. These phenomena are understood qualitatively, but only simulations can provide quantitative estimates of the relative importance of the various effects in realistic situations.

Synergia is a package based on IMPACT, a code originally developed at Los Alamos to study space-charge induced halos in high intensity linacs. A substantial part of the code has in fact been re-used, and the Synergia team wrote "glue" components, reducing development cost. Despite the technical difficulties encountered in assembling Synergia from components originating from different sources and implemented in different languages, the committee is supportive of the approach. An advantage is that users can begin using the code immediately while the team continues to acquire experience.

In addition to writing a simulation package, Panagiotis Spentzouris and Jim Amundson have also conducted experiments at the Booster and compared the results with their simulations. They should be commended for a significant amount of high quality work. Very nice preliminary results were shown.

The Synergia team has, in a relatively short time, had a significant influence on some Booster operational issues. They communicate regularly and collaborate closely with Beams Division personnel. This type of collaboration has historically been difficult to accomplish and should be supported. Simulation of space charge effects is important not only for existing machines like the Booster, but also for possible future high intensity proton synchrotrons. Participation of the laboratory in SciDAC is important in terms of scientific contributions to the field of computational accelerator physics and in terms of the establishment of a critical mass of local expertise. Such expertise is important for the study of future projects and also will determine in large measure how successful the Laboratory will be in attracting future government funding for computational activities.

Specific responses to the charge

Here are the responses to the specific issues raised in the charge to the committee:

[1] Are the simulation techniques used in Synergia appropriate for evaluating space charge in the Booster and other circular machines?

The simulation techniques are sound. The space-charge algorithm used in Synergia/IMPACT is well established and suitable to run on large parallel systems: the electric potential is calculated in the beam frame by convolution of a free-space Green's function with the bunch charge distribution. The convolution itself is performed using 3D FFTs.

While the convolution algorithm is certainly appropriate, one should not get the idea that this is the only competitive method available (the Fast Multipole Method is an example of another viable algorithm). One issue is that in order to preserve accuracy, the spatial discretization must be performed on a relatively uniform grid. Since bunches in circular machines are typically much longer than their transverse size and since it is important to model the details of the potential variation along the transverse dimension, a correspondingly high sample density is required in the longitudinal dimension, substantially increasing computation time. The developers of IMPACT have recently attempted to improve the algorithm by using special non-Fourier longitudinal expansions, but so far, the reported performance has been disappointing. Computational efficiency is an important issue for simulations over a complete acceleration cycle. For example, a single Booster turn with a million macroparticles currently represents about an hour of computer time on a modest number of processors (8-16). Granted that transverse space charge effects are most important early in the cycle, still the beam makes about 20,000 turns during an entire acceleration cycle in the Booster.

[2] A well-planned validation with data is critical for any simulation program. Has the validation program using Booster IPM data resulted in a useful test of the Synergia simulation package?

Panagiotis and Jim have done a very good job of understanding, calibrating, and using the Ion Profile Monitor in the Booster. The IPM measures the transverse beam size distribution, and hence indirectly the emittance, by collecting ions created by the passage of the beam through the residual gas. In the presence of space charge, one expects the emittance to grow with a rate that increases with beam intensity. This is a direct and observable measurement of the effect of space charge.

Numerically, insufficient macroparticle statistics cause "artificial" emittance growth that must be distinguished from real emittance growth. This may be a problem when growth due to physical mechanisms is already relatively small. The IPM is not necessarily the best device to observe the tails of the beam distribution, the halo region, with sufficient resolution. Another problem is that the relative gains of the channels where the ions are collected vary. Typically, the channels that receive the most ions have a reduced gain.

The main challenge for interpreting IPM data is that the ions do not travel in parallel paths to the collection grid. Rather, the beam self-field causes the trajectories to curve. As a result the measured transverse profiles are distorted in an intensity-dependent way. A correction must be computed and applied a posteriori. To compute the correction, one must necessarily make an initial assumption about the (unknown!) beam shape. The analytical and numerical work of the Synergia team has led to a much improved IPM correction algorithm.

The committee (favorably!) views the comparison of Synergia results with Booster IPM data primarily as the (successful!) beginnings of an attempt to do physics rather than a software validation program. The effort to simulate a real machine like the Booster is a powerful motivator for the addition of needed features to the software. The Booster study results might also be construed as evidence for the validity of Synergia. However, the Booster is too complicated and not well enough understood to provide convincing code validation. Also, there are large uncertainties in the measurements and in the knowledge of beam initial conditions. The IPM is a relevant diagnostic; however, good agreement with IPM data should not be regarded as a conclusive test.

The Synergia team should participate in the overall SciDAC code validation program. This is in their work plan, and they should be strongly encouraged to do so, even if such validation programs have already been run on IMPACT, or have no direct bearing on the Booster performance. Such validation tasks not only are crucial to keep re-assessing the validity of Synergia as it keeps evolving, but also will strengthen their reputation in the accelerator simulation community. These validation tests should also be maintained and documented as "potential examples".

At an ICFA Mini-Workshop in Oxford, England in April of this year, several of the participants agreed to a joint effort on space charge code benchmarking. Data from a CERN PS experiment on the Montague resonance will be used. The Synergia team should take part in this comparison activity.

It would also be important to validate the code using some standard simple cases. The most obvious one would be a simulation of a beam with a K-V distribution propagating in a continuously focusing machine. In that case, all the space charges forces are linear and calculable. The steady state solution is an unstable equilibrium.

[3] Have sufficient beam studies with the Booster been made?

The data acquired so far during dedicated beam study periods have proven very useful for stimulation of code development and then for comparison with Synergia results. However, dedicated Booster beam study time is a scarce commodity. More Booster beam studies are warranted, but pragmatism requires that most future studies be parasitic. Parasitic study time is readily available, but such studies cannot deviate too much from normal running conditions. That is not much of a limitation because those are the most interesting conditions anyway if the goal is to understand the real machine.

In particular, “normal running conditions” means magnets ramping and rf cavities accelerating. Although acceleration has been implemented in Synergia, much of the data and Synergia simulations to date have been performed with magnet currents DC and rf off. Future studies should involve mostly parasitically acquired data during normal acceleration cycles with rf on. The effects of varying the intensity and other parameters early in the cycle should be studied under those conditions. Once there is confidence in the ability to properly handle acceleration, then transition crossing could also be studied. Although longitudinal space-charge effects at transition are well known, the possible interaction of transverse and longitudinal effects at transition is virgin territory.

[4] Are the extrapolations to high intensity operation scenarios valid?

The committee is not in position to answer this question regarding the specific work under review because the Synergia team did not present numerical results related to high intensity extrapolations to the full committee. (A private conversation with one committee member after the presentations revealed that they actually ran the code at higher intensity and saw more halo created, but did not present quantitative results because no experimental data are available for comparison.)

Although the committee lacks specific information regarding Synergia extrapolations to high intensity, some general comments are in order. A machine like the Booster is a complex object. Space charge is only one of several factors influencing performance. A complete model would include various magnetic field errors at injection (remanent fields), field defects due to saturation, magnet alignment errors, beam coupling impedances, the effects of transition crossing and coherent instabilities, and so forth. All these factors must be studied both separately and concurrently, as they can sometimes conspire. Reliable quantitative predictions about performance at intensities well beyond current experience would require a model that not only incorporates all the important physics but also includes correct "initial conditions" such as an accurate knowledge of field errors. At the present state of the art, quantitative agreement of such predictions with reality would probably be fortuitous in most cases.

Nevertheless, the committee believes that Synergia will be quite useful for understanding the role played by space charge in high intensity circular accelerators. The results of such simulations are particularly valuable for guiding design decisions for future accelerators and upgrades of existing ones. Such design decisions can be based on the relative performance of various possibilities, even if the absolute predictions are uncertain.

[5] Is the software suite user-friendly and efficient?

As mentioned above, the algorithm at the heart of Synergia is a standard and well-established one. Efficiency in a parallel context is a matter of dynamically balancing the load on each processor. IMPACT load balancing has been carefully optimized over the years.

Panagiotis and Jim have made significant efforts to integrate existing software components. The technique employed, a python wrapper communicating through files, was the most expeditious choice. Although the committee has not tried to use the software, the presentations suggested that running Synergia should be a straightforward matter for a knowledgeable person.

Because Synergia is a mixed language package (f90/C++/python), some increased complexity in terms of installation, support and maintenance is to be expected. That should not be a serious issue; furthermore, a reasonable plan was presented for better integration of the python front end in the future. Some web-based documentation is already available and needs to be expanded.

[6] Please comment on the plans for further simulations and studies.

In addition to the measures embodied in the discussions above, the committee recommends that the Synergia team pursue the following future activities. The.key words here should be consolidation and strengthening via a vigorous program of Booster studies and software augmentations.

Regarding simulations, a plan for rewriting the main IMPACT loop has been presented and looks good. The Synergia team should consider rewriting this main loop in C++ rather than Python, thereby restricting the usage of Python to the interface between the input script and the core package, because this main loop may contain more interfaces than presently foreseen, and C++ looks more appropriate for such a "framework" task.

As previously emphasized, the ability to simulate acceleration must be established. (This is implemented at some level, but has not been extensively tested.) RF capture, transition phase jumps, and energy dependent field errors should be included. Also, Synergia could possibly be expanded to include more realistic machine impedances.

Improved numerical diagnostics should be implemented. This is important, since at the moment Synergia provides only phase space coordinates for all particles. To compare with experimental and theoretical results, users expect to be able to compute moments at various locations around the ring through an acceleration cycle. This can be done offline by dumping phase space data periodically, but that arrangement is cumbersome. Another important diagnostic is the ability to produce single particle tune footprints since those can be correlated with theoretical results.

Regarding beam studies, a comprehensive long-term plan that emphasizes parasitic studies should be developed.

After the present shutdown a vertical IPM will be available in addition to the previously used horizontal one. The horizontal beam profiles are complicated because they reflect both transverse radial and longitudinal phase space distributions. Separating out the evidence for transverse emittance growth from the effects of the rapidly evolving momentum distribution is an interesting challenge. However, interpretation of the vertical profiles in terms of space charge induced emittance growth will be more straightforward.

The Synergia team should also develop a coherent plan to consolidate their analysis and studies. In particular, so far they have avoided drawing definite and quantitative conclusions regarding the emittance dilution due to space charge in the Booster as a function of time and intensity. Various plots show that information implicitly. However, a quantitative and conclusive summary, with a serious attempt at determining the systematic errors in both measurement and simulation, could be written up. Maybe they need more beam studies to reach that stage. If so, they definitely deserve the necessary support for conducting such studies.

Finally, the idea of adding a graduate student or postdoc to the Synergia team was briefly discussed. Such an expansion is warranted not only because the project would make faster progress with more manpower, but also because the activity would be very educational. The committee encourages lab management to seriously consider that possibility.